BUBBLE NUCLEATION IN φ^4 MODELS AT ALL TEMPERATURES

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Abstract

One possible way in which phase transitions in the early universe may have ocurred is via nucleation of bubbles of the new phase (true vacuum) in the old phase (false vacuum). The technique most widely used to compute the probability of bubble nucleation is based on instanton methods in the context of the semiclassical approximation. At zero temperature in 3+1 dimensions the nucleation rate is dominated by the O(4) symmetric instanton, a sphere of radius R, while at temperatures $T >> R^{-1}$, the decay is dominated by a "cylindrical" (static) instanton wtih O(3) invariance. There has been discussion in the literature as to whether the transition between these two regimens would be first order (discontinuity in the first derivative of the nucleation rate at the transition temperature T_c), or second order (continuity of the first derivative, but discontinuity of the second derivative at T_c). In this paper we obtain the finite temperature solutions corresponding to the quantum and the thermal regimes, and compute their action as a function of the temperature for different values of the wall thickness in a φ^4 potential. Our results indicate that only for the cases of very large wall thickness a second order transition takes place, while for all the other cases a first order transition occurs.

1   Introduction

The problem of the decay of a metastable state via quantum tunneling has important applications in many branches of physics, from condesed matter to particle physics or cosmology. In many cases however, the difficulties associated with a full quantum treatment, and the fact that tunneling is a non-perturbative effect, make it impossible for us to be able to make quantitaive predictions about the behaviour of the system. When the nature of the tunneling system allows the use of the semiclassical approximation though, instanton techniques, used to describe quantum tunneling in that regime, provide us with a formalism capable of producing accurate values for decay rates. In condesed matter this formalism has been applied to an array of problems ranging from the tunneling of an Abrikosov vortex line out of a pinning potential in a superconductor [1-3], to the change in the magnetization direction of thin films under field inversion [4]. In the context of cosmology, perhaps the most compelling example is that of the study of first order phase transitions in the early universe [5], although other problems such as the decay of metastable topological defects formed during these transitions [6], have also shown to be amenable to this sort of treatment.

The basic tenet of the formalism is that the decay rate per unit time (and where applicable per unit volume) is given by an expression of the form

$$\Gamma = A e^{-S_E} \tag{1}$$

where S_E is the Euclidean action of the instanton: the classical solution to the equations of motion under the potential barrier in euclidean time with periodic boundary conditions. The instanton has turning points at the configurations at which the system enters and exits the barrier, and its analytic continuation to Lorentzian time at the exit point describes the appearance of the system at the other side of the barrier and its subsequent evolution. When the solution for the given boundary conditions is not unique, one should take into account only the one with the lowest S_E, which will dominate (1) (unless of course all or some of the solutions happen to have comparable actions, in

which case one should take all relevant contributions to Γ into account). The determinantal prefactor A in Eq.(1), meanwhile, results from a gaussian functional integration over small fluctuations around the instanton. The formalism was first developed and applied to false vacuum decay at zero temperature in refs [7-9]. The dominant solution in this case is a maximally symmetric instanton invariant under O(4) (for three spatial dimensions) [9].

In the context of quantum mechanics (i.e. $0+1$ dimensions) the formalism was extended to include finite temperature effects by Affleck [10]. Under certain assumptions for the shape of the barrier he found that above a critical temperature determined by the curvature of the potential at the top of the barrier, the dominant solution was a "static" (euclidean time independent) instanton sitting at the bottom of the inverted potential well, the decay rate produced by this solution recovering the expression for purely classical thermal activation over the barrier that we would expect to dominate the procces at high temperatures. The transition between the thermal and quantum regimens is dominated by solutions with a finite period in the Euclidean time that smoothly interpolate between the zero temperature instanton and the "static" high temperature solution. The transition is thus a second order one (i.e., the decay rate Γ and its first derivative with respect to the temperature are continous at the critical temperature of the transition, T_c, but not so the second derivative).

Chudnovsky [11] however showed that this situation is not generic, and that the type of transition will in general be determined by $d\tau_p/dE_{eucl}$, the derivative of the euclidean period of the motion τ_p with respect to its euclidean energy. For the case in which the period vs. energy curve possesses a minimum at values of (E_{eucl}, τ_p) different from those associated with small oscillations around the minimum of the potential, it can be shown that, at the transition temperature, the dominant solution changes discontinously to the high temperature instanton. Consequently the curves for the actions of both regimens cross each other at that point, and the derivative of S_{min} with respect to the temperature (and thus that of Γ) changes discontinuosly as we go from the thermal activation regime to the quantum regime. This is what Chudnovsky called a *first order* transition. In this

case we should be able to observe quite a sharp change in the behaviour of Γ as we go through the critical region.

In the context of field theory very little work has been done towards examining the structure of the intermediate regime instantons as well as that of the transition between the two extreme cases of high and zero temperature. Studying the bubble nucleation rate for phase transitions in the early universe, Linde [5] suggested that periodic instantons would smoothly interpolate between these two regimens, much in the same way that Affleck had shown could be the case for quantum mechanics shortly before. In this picture then, one would have Coleman's O(4) invariant spherical bounce of radius R dominating at zero temperature. As one goes into finite temperature one would first encounter a periodic array of, rather weakly interacting, widely separated spheres, but after we have increased the temperature up to values $T \sim (2R)^{-1}$ and beyond we no longer can fit the spheres into the corresponding periods, and they would start merging into one another producing what has become known as a "wiggly cylinder" solution. As we keep increasing the temperature further, the wiggles eventually smoothly straighten out, and the solution goes into the O(3) invariant "cylinder" that dominates the thermal activation regime.

In correspondence with the work of Chudnovsky in quantum mechanics however, Garriga [12], in a recently published paper, has shown that within the thin wall approximation the transition is in fact not second order, but rather, first order. The wiggly cylinder solutions do indeed exist within some range of the temperature, but when they exist they always have a higher action than any of the other solutions for the same temperature, and therefore they never dominate the exponential in (1). The instanton that saturates (1) goes then abruptly from being a periodic series of separated bounces to being the cylindrical solution, and the rate of change of the action with the temperature changes discontinuosly. The transition thus produced is in consequence first order. It may be worth noting at this point that the terminology used to describe this transitions (i.e., first and second order) refers *only* to the type of transition between the two different instanton regimes, and not to

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the phase transition of the physical system itself.

In this paper we aim to explore the nature of the transition between the thermal hopping and the zero temperature regime when we go beyond the thin wall approximation, in the context of the bubble nucleation problem in φ^4 models just mentioned. In order to do this, we will develop an algorithm to numerically compute the relevant finite temperature solutions for a given value of f (the parameter that governs the width of the wall as compared to the radius of the bubble), and then compute the corresponding curve for the action as a function of temperature. Finally we repeat this procedure for different values of f, covering the most significant physical cases. Our results indicate that in the case of extremely thick wall (when the tunneling occurs over a very shallow barrier) we do get a second order transition, but that in all other cases the transition is in fact first order, in particular,close to the thin wall regime our results agree rather well with those of Garriga. In spite of the fact that in any realistic model of the phase transition the potential will be temperature dependent, whereas we use temperature independent potentials, we do not expect this to significantly change our results, as will be seen at the conclusion. The paper is organized as follows: in section II we give a quantitative account of the finite temperature transition in the spirit of [11], in section III we present the results that Garriga obtained for bubble nucleation in the thin wall limit, in section IV we introduce our numeric algorithm and in section V we present our results. Finally, conclusions are in section VI

2 Finite Temperature Instantons in Quantum Mechanics

Acording to [7] the decay rate in the semiclassical limit ($S >> \hbar$) is,

$$\Gamma \propto exp(-S_{min}/\hbar) \tag{2}$$

where $S_{min}(T)$ is evaluated along the $q(\tau)$ trajectory with period $\tau_p = \beta = \hbar/k_B T$ that minimizes the Euclidean time action

$$S(T) = \int d\tau \mathcal{L} = \int d\tau [\frac{1}{2} M\dot{q}^2 + V(q)] \quad , \tag{3}$$

with $\dot{q} = dq/d\tau$ and where the integral is performed over a whole period β (see [7-9], [11] for details; from now on we will use β to designate both the euclidean period and the usual inverse temperature). Such trajectories will of course be solutions of the classical equations of motion in Euclidean time

$$M\ddot{q} = \frac{dV}{dq} \tag{4}$$

consistent with the boundary conditions, that is, periodicity with period β. (i.e., $q_1 = q(-\beta/2) = q(\beta/2)$ and $q_2 = q(0)$ will be the turning points of the motion). By noting that (4) is the equation of motion of a particle in a potential -V in Lorentzian time, we can draw two consequences: first, that the (positive) energy

$$E(\beta) = V(q) - \frac{1}{2} M\dot{q}^2 \tag{5}$$

is conserved. And, second, that by inverting the barrier we can recognize the types of solutions that we will have for the motion of the particle in the well (see Fig. 1). It is then immediately obvious that there are two solutions with period β, one that actually is a time independent solution sitting at the bottom of the well, $q = q_0$, and another one that corresponds to periodic motion in the inverted well between $q_1(E)$ and $q_2(E)$. For the first one we will have from (3) an action

$$S_0 = V(q_0)\beta \quad , \tag{6}$$

whereas for the second one, use of (5) into (3) yields

$$S_T = 2(2M)^{1/2} \int_{q_1}^{q_2} dq[V(q) - E]^{1/2} + E\beta \quad , \tag{7}$$

where E and β are related through

$$\beta = (2M)^{1/2} \int_{q_1}^{q_2} dq[V(q) - E]^{-1/2} \quad . \tag{8}$$

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Then, from (6), (7) and (8) one obtains

$$\frac{dS_0}{d\beta} = E_0 \ , \qquad \frac{dS_T}{d\beta} = E > 0 \quad , \tag{9}$$

and

$$\frac{d^2 S_0}{d\beta^2} = 0 \ , \qquad \frac{d^2 S_T}{d\beta^2} = \frac{1}{d\beta/dE} \quad . \tag{10}$$

The behaviour of these derivatives at the temperature T_c at which $S_T = S_0$ will then determine the type of transition between the two regimens: if at T_c we have $S_0' \neq S_T'$ the transition will be first order, but if the equality holds, we will have a second order transition for which $S_0'' \neq S_T''$ as we are about to see. From (10) however we see that this will in turn be determined by the behaviour of $d\beta/dE$ (which can be interpreted as the specific heat of the system).

As a first example we can look at potentials of the form $-q^2 + q^3$ or $-q^2 + q^4$ [10]. In this case β monotonically decreases with E (Fig. 2), until it eventually reaches β_0, the period of small oscillations at the bottom of the potential. As seen from Fig.2, $S_T \to S_0$ and $S_T' \to E_0 = S_0'$ as $\beta \to \beta_0$, or what is the same, as $T \to T_0$, $T_0 (= \hbar/k_B \beta_0)$ being the transition temperature in this case. The second derivative S_T'' will however change discontinually as we go across T_0, and will, as a matter of fact be undefined at that temperature (of course a more careful quantum analysis is needed at this point). This is what Chudnovsky called a second order transition.

The other case of interest to us is that for which $\beta(E)$ develops a minimum, at say (E_1, β_1), before reaching β_0 at E_0 (see Fig.3). This will be the case for potentials that change very slowly both at the top and the bottom (although still being parabolic) but that are very steep in the middle. In this case we see that, as E decreases from E_0 to E_1, we have $S_T' = E < E_0 = S_0'$ and $S_T'' = 1/\beta' > 0$. The corresponding curve for $S_T(\beta)$ will then be a concave curve that stays always above the thermal activation curve. At E_1 however $\beta' = 0$ and S_T'' is undefined, and for $E < E_1$ we have to have a convex curve that quickly goes into a straight horizontal line for high vlaues of β (Fig. 3b). S_T then has to cross over the S_0 curve at some period β_c. The derivatives of the two curves will be different at that point and, therefore, the first derivative of S_{min} will suffer a

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discontinous change as we go across the corresponding critical temperature $T_c = \hbar/k_B\beta_c$ (note that $T_0 < T_c < T_1$), producing thus a first order transition.

3   Finite Temperature Instantons in Field Theory

Studying first order phase transitions in the early universe, Linde [5] suggested an extension of the previously discussed second order transition scenario (published by Affleck shortly before) to the field theory case. Due to spherical symmetry in the spatial coordinates, the equation of motion for the field is now

$$\frac{\partial^2 \varphi}{\partial \tau^2} + \frac{\partial^2 \varphi}{\partial r^2} + \frac{2}{r}\frac{\partial \varphi}{\partial r} = \frac{\partial V}{\partial \varphi} \quad , \tag{11}$$

where r is the spherical radial distance. We will choose the potential to be of the form:

$$V(\varphi) = \frac{\lambda}{2}(\varphi^2 - \mu^2)^2 - F\varphi \quad . \tag{12}$$

As for the boundary conditions, in the r direction the requirement of finite action leads to $\varphi \to \varphi_+$ as $r \to \infty$, while in the τ direction periodicity alone no longer suffices, and we have to impose that the configurations at $\tau = \pm\beta/2$, 0 have zero derivative along the τ direction to ensure that they are indeed turning points. We thus have

$$\varphi \to \varphi_+ \text{ as } r \to \infty \ , \quad \partial\varphi/\partial\tau = 0 \text{ at } \tau = \pm\beta/2 \ , \ 0 \quad , \tag{13}$$

where β is the period of the solution. The idea is then that the relevant solutions should follow the same lines as above: at low temperatures the solution would be a periodic array of widely separated O(4) spherical bounces (with radius R). As we go into temperatures $T \geq (2R)^{-1}$ however we no longer can fit a bounce in each period and they start merging into one another, forming an oscillating "wiggly" cylinder analogous to the oscillating solutions of the quantum mechanical case. These wiggles would then subsequently smooth out as we increase the temperature and eventually disappear at temperatures $T >> R^{-1}$, providing a smooth transition into the "cylindrical" (τ

independent) instanton corresponding to the thermal activation regime. Fig.4 shows this sequence. As we increase the temperature, the transition would be then a second order one.

As noted in the introduction however, Garriga [12] has shown that at least in the thin wall approximation this is not the case. In this approximation, the parameter F in the potential above (and correspondingly the energy difference between the two different phases, $\epsilon = 2F$) is very small, and as a consequence the width of the wall separating the bubble of true vacuum from the false vacuum is very small compared to its radius R (i.e., one needs a larger bubble to compensate for the wall energy). In Lorentzian time then, the dynamics of the bubble can adequately be described by an effective action (in 3 spatial dimensions)

$$ S = -\sigma \int d^3\xi \sqrt{\gamma} + \epsilon \int dV dt \quad , \tag{14} $$

where the first term is the Nambu action proportional to the area of the world sheet of the wall (σ being the wall tension, ξ^a a set of coordinates on the world sheet and γ the determinant of the world sheet metric), while the second is the volume of the bubble times the energy difference between the two phases integrated over time. With a flat background geometry, adopting spherical coordinates and a spherical ansatz for the world sheet means that we can write S as

$$ S = -\sigma \mathcal{S}_2 \left[\int r^2 (1 - \dot{r}^2)^{1/2} dt - \frac{\epsilon}{3\sigma} \int r^3 dt \right] \quad , \tag{15} $$

where $\dot{r} = dr/dt$ and $\mathcal{S}_2$ is the surface of the unit sphere. Since the Lagrangian does not depend on time, the energy

$$ E = p_r \dot{r} - L = \sigma \mathcal{S}_2 \left[\frac{r^2}{(1 - \dot{r}^2)^{1/2}} - \frac{\epsilon}{3\sigma} r^3 \right] \quad , \tag{16} $$

must be conserved. With a little algebra this can be written as

$$ \dot{r}^2 + V(r, E) = 0 \quad , \tag{17} $$

where

$$ V = \left[\frac{E}{\sigma \mathcal{S}_2} r^{-2} + \frac{\epsilon}{3\sigma} \right]^{-2} - 1 \quad , \tag{18} $$

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The instantons relevant to the problem are then found by performing a Wick rotation in (17), whence we obtain

$$\dot{r}^2 - V(r, E) = 0 \quad , \tag{19}$$

where now $\dot{r} = dr/d\tau$. There are two types of solutions to (19) depending on the value of E: for $E = 0$ and $\beta \to \infty$, the solution is just Coleman's bounce with radius $R = 3\sigma/\epsilon$, and action

$$S_T = \sigma \mathcal{S}_3 R^3 / 4 = \sigma \pi^2 R^3 / 2 \quad . \tag{20}$$

Keeping $E = 0$ but introducing a finite value for β produces then a periodic array of bounces in the τ direction. These solutions exist for as long as $T \leq T_* = (2R)^{-1}$ and will continue to have the same action S_T, since outside R the field decays exponentially. For $E > 0$ though, the inverted potential -V takes the form of a well and the motion of r in it acquires two turning points, r_{min} and r_{max}. The solution is then wiggly cylinder shaped. If we keep increasing E, $-V$ becomes shallower and shallower, and the two turning points start approaching each other until they eventually merge at values E_0, r_0. From the condition $V(r_0, E_0) = V'(r_0, E_0) = 0$ ($V' = dV/dr$), we get values for the radius of the cylinder

$$r_0 = \frac{2}{3} R \quad , \tag{21}$$

and its corresponding energy

$$E_0 = \frac{4\pi r_0^2}{3} \sigma = \frac{16\pi}{27} \sigma R^2 \quad . \tag{22}$$

Since it is static, the solution $r = r_0$ will exist at all temperatures, and its Euclidean action

$$S_0 = E_0 \beta \tag{23}$$

will be proportional to the period (= temperature^{-1}). This will therefore be the dominant solution at high temperatures.

It suffices now to compare S_T and S_0 to see that there will be a temperature for which $S_T = S_0$, namely

$$T_c = \frac{32}{27\pi} R^{-1} \quad . \tag{24}$$

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At this temperature then, the curves for S_0 and S_T will cross each other, and consequently the slope of the curve that follows the minimum action S_{min} will change discontinously. The transition between the two regimes is thus first order. It can be shown (see Ref.12) that the wiggly cylinder solutions that exist for $0 < E < E_0$, do, as a matter of fact, always have greater actions than either the periodic array of bounces or the static cylinder, and therefore never dominate S_{min}.

The question that we aim to answer is then the following: Is this situation general for bubble nucleation, or will we find a second order transition as suggested by Linde when we go into the thick wall case?.

4   Algorithm

We start with the Euclidean action

$$S_E = 4\pi \int d\tau \int dr r^2 \left[\frac{1}{2}(\dot\varphi^2 + \varphi'^2) + \frac{\lambda}{2}(\varphi^2 - \mu^2)^2 - F\varphi \right] \quad, \tag{25}$$

where $\dot\varphi = \partial\varphi/\partial\tau$, $\varphi' = \partial\varphi/\partial r$. We then rescale the Lagrangian

$$\varphi \to \varphi/\mu \quad, \quad \tau \to \tau\sqrt{\lambda\mu^2} \quad, \quad r \to r\sqrt{\lambda\mu^2} \quad, \quad f = F/(\lambda\mu^3) \quad, \tag{26}$$

to get

$$S_E = \frac{4\pi}{\lambda} \int d\tau \int dr r^2 \left[\frac{1}{2}(\dot\varphi^2 + \varphi'^2) + \frac{1}{2}(\varphi^2 - 1)^2 - f\varphi \right] \quad. \tag{27}$$

The only adjustable parameter in the Lagrangian is now f, so by covering its whole range we should be covering all relevant cases. The equations of motion are now

$$\frac{\partial^2\varphi}{\partial\tau^2} + \frac{\partial^2\varphi}{\partial r^2} + \frac{2}{r}\frac{\partial\varphi}{\partial r} = \frac{\partial V}{\partial\varphi} = 2(\varphi^3 - \varphi) - f \quad, \tag{28}$$

and the boundary conditions are the usual ones

$$\varphi \to \varphi_+ \text{ as } r \to \infty \quad, \quad \partial\varphi/\partial\tau = 0 \quad \text{at} \quad \tau = \pm\beta/2, 0 \quad. \tag{29}$$

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To solve this equation we have used a multigrid algorithm. Multigrid methods were first introduced in 1970s by Brandt [13] (see also [14] for a brief introduction and further bibliography on the subject), and the basic underlying idea is the following: let's suppose that we have to solve a linear equation of the form

$$L_h(q_h) = 0 \quad , \tag{30}$$

where L is some discrete form of the linear differential operator, q is the discrete solution, and the subscript h denotes a discretization of the independent variables (i.e., τ and r in our case) in a mesh with meshsize h. In order to do this, iterative methods usually start with an approximate solution $\tilde{q}_h$ such that

$$L_h(\tilde{q}_h) = d_h \quad , \tag{31}$$

where d_h is called the *defect*. We then look for approximate solutions, $\tilde{v}_h$, of

$$L_h(v_h) = -d_h \quad , \tag{32}$$

to form

$$\tilde{q}_h^{new} = \tilde{q}_h + \tilde{v}_h \quad . \tag{33}$$

$\tilde{q}_h^{new}$ will then be closer to the true discrete solution q_h than what $\tilde{q}_h$ was. Under some general conditions for the form of the matrix of coefficients of the discretized algebraic equations, iteration of this procedure is a convergent process, converging upon q_h. The heart of the matter is then what approximation to use to solve (32) and find $\tilde{v}_h$.

As an example we have relaxation methods, where what one does is to replace L_h in (32) by a *simpler* operator (such as just its diagonal part for instance), and then solve the set of equations. The drawback here however is that, as solving the set of discretized equations is basically a point by point procedure, convergence for the long wavelenght modes of the solution will be rather slow usually.

Multigrid methods operate by *coarsifying* rather than *simplifying* the problem. Instead of solving the problem in a mesh of size h with a simpler operator, we *project* the problem into a coarser grid

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of size H, solve there for $\tilde{v}_H$ and then *interpolate* back to find the corrections $\tilde{v}_h$ in the finer grid. Appart from having to solve far less equations than in the finer grid, transfering to a coarser grid has the added advantage of dramatically improving the convergence rate of the long wavelenght modes. However, if applied as such, this process will not only not converge, but slightly diverge for short wavelength modes. What one does then is to apply one or more realaxation sweeps before and after transfering to the coarse grid, to smooth out the short wavelength componenets of the error that relaxation handles so well.

Several developments on this basic scheme are now possible. In first place, it is obvious that nothing prevents us from adding more grids to the algorythm, going each time to coarser and coarser meshes. In principle nothing prevents us in fact from going to grids so coarse that we only have to solve a handful of equations. Starting from such a grid and computing in it not just the correction, but the full solution $\tilde{q}_H$, and then going up the ladder and so on, eliminates the need for having an initial guessed solution fed into the algorythm. This is known as the full multigrid method.

Another possible expansion leads to an algorithm that can solve non-linear problems. In this case, if we have to solve

$$L_h(q_h) = f_h \quad , \tag{34}$$

where f_h is some right-hand side term, we need a smooth correction v_h to the current solution $\tilde{q}_h$ so that

$$L_h(\tilde{q}_h + v_h) = f_h \quad . \tag{35}$$

To do this note that

$$L_h(\tilde{q}_h + v_h) - L_h(\tilde{q}_h) = f_h - L_h = -d_h \quad . \tag{36}$$

Transfering this equation to the coarser grid after the pre-relaxation sweeps leads to

$$L_H(q_H) - L_H(\mathcal{R}_H^h \tilde{q}_h) = -\mathcal{R}_H^h d_h \quad , \tag{37}$$

where $\mathcal{R}_H^h$ is the restriction operator from gridsize h to gridsize H. That is, in the coarse grid we

solve for

$$L_H(q_H) = L_H(\mathcal{R}_H^h \tilde{q}_h) - \mathcal{R}_H^h d_h \quad . \tag{38}$$

If the approximate solution is then $\tilde{q}_H$, then the coarse grid correction is

$$\tilde{v}_H = \tilde{q}_H - \mathcal{R}_H^h \tilde{q}_h \quad , \tag{39}$$

and the corrected fine grid solution will then be given by

$$\tilde{q}_h^{new} = \tilde{q}_h + \mathcal{I}_h^H \tilde{v}_H \quad , \tag{40}$$

where $\mathcal{I}_h^H$ is now the interpolation operator between gridsize H and gridsize h. Note that in general $\mathcal{IR} \neq 1$, and so $\tilde{q}_h^{new} \neq \mathcal{I}_h^H \tilde{q}_H$.

For our problem we used full weighting injection for the projection operator (see Ref.14) and second order polinomial interpolation (fourth order for the thin wall case). We were precluded from using a full multigrid approach because we encountered a bifurcation problem. This problem can appear in cases where the non-linear equations have more than one solution compatible with the boundary conditions, and in practice it means that for certain values of the mesh size h the coefficients of the discretized equations blow up. One is therefore confined to using meshsizes smaller than that for which the problem appears, and does not have acces to a mesh coarse enough to be able to solve the equations exactly. To solve this problem we limited our algorythm to use only three meshes. As for the needed initial guess solution, what we did was to obtain the zero temperature profile of the bounce via a simple shooting routine (remember that at zero temperature the dominant solution is $O(4)$ symmetryc, and therefore the problem can be reduced to a 1-dimensional differential equation). We then put it in a two-dimensional form and fed it to the multigrid algorithm. After computing the form of the zero temperature solution in this way we then proceeded to compute finite temperature solutions by continuation in the temperature (i.e., using the previous solution as the guess for the next one with slightly higher temperature).

Since Zebra relaxation turned out to be unstable for our problem, we used line Newton-Jacobi in the τ direction for the relaxation smoother (as increasing the temperature meant in practice reducing the mesh size in that direction). Special care had to be taken to handle the negative modes of the instantons. One of the general conditions that relaxation methods need to converge is the absence of eigenvalues with opposite signs in the diagonalization of the matrix of coefficients. Instantons however do have a negative mode in their perturbation spectrum, as they describe unstable states. Since at any point relaxation amounts to solving the linearized equations for the correction around the present value of the solution, a relaxation procedure is bound not to converge. To take care of this problem what we did was to fix the value of the field at the center of the instanton, φ_c. (What this means in practice is that after each relaxation step we multiply the whole solution by a constant so that the center remains at the desired value without breaking the continuity of the relaxation process around it). The problem is then equivalent to that of a membrane with the center and the boundaries fixed to a certain value and subject to a potential, which should make it stable unless we have choosen too high a value at the center. In that case, the whole membrane will want to jump over the potential barrier (i.e., in the language of Ref. 7 we will be overshooting). Thus, if the value for φ_c is too high the solution will still diverge, but if it is below critical relaxation should converge. At the boundary between these two cases should lie then the true value of the instanton at its center, φ_{Tc}, and fixing φ_c to this value should make the relaxation of the instanton a convergent process.

We tried this procedure with the zero and high temperature solutions, where we could get independent figures for φ_{Tc}, with a much higher precision from the shooting routine (since in both limits the equation of motion turns into a simpler differential equation). In practice we found that if the value chosen for φ_c was too high by an amount say Δ (so that $\varphi_c - \varphi_{Tc} \sim \Delta$) the solution would start first by converging up to an overall accuracy level roughly of the order of Δ, and only *after* reaching that accuracy level would it start to diverge. Thus it usually didn't take long to produce a value for φ_c within a 0.1% difference from the φ_{Tc} value given by the shooting routine,

and a correspondingly low level of error for the whole solution.

5   Results

Using this algorithm then we aim at finding all the relevant finite temperature solutions of the equations of motion

$$\frac{\partial^2\varphi}{\partial\tau^2} + \frac{\partial^2\varphi}{\partial r^2} + \frac{2}{r}\frac{\partial\varphi}{\partial r} = \frac{\partial V}{\partial\varphi} = 2(\varphi^3 - \varphi) - f \quad , \tag{41}$$

to elucidate whether the transition between the thermal hopping and the low temperature regimens is first or second order. We will do this for three different values of the parameter f. The first value that we will take for f will be chosen so as to check our procedure against Garriga's predictions for the thin wall case. Although in order to do this it would be desirable in principle to pick a value for f as small as possible so that we get a wall as thin as possible, practical considerations limit how small a value for f we can choose. Since in the thin wall limit the wall radius is proportional to f^{-1}, the smaller the value of f the larger the mesh that we would need to cover the whole bubble. But at the same time we need to have the mesh size small enough so that it can adequately represent the structure of the wall in a smooth way. Clearly then, if we do not want to have so many points in the mesh that the whole algorithm becomes unmanageable, there is a limit as to how small we can set the value of f. It turns out however that for our pourposes $f = 0.25$ is more than adequate.

For such a value of f, we get a wall about half as thick as the interior of the bubble. Fig.5 represents the shape of the potential for this case, an Fig.6 shows several finite temperature solutions. To compute the action of each solution we used a two dimensional version of the Romberg integration code that can be found in Ref. 14. When comparing the results obtained in this way with those provided by the shooting routine for zero temperature and the thermal hopping regimes, we consistently found a difference of about 0.2% of the total value. We feel that a conservative stimate for the error in the value of S_E at each point should then be no higher than 0.5%. Fig.7 gives us the S_E vs. T dependence. From it we can deduce an approximate value for the temperature

T_c at which the transition takes place of $T_c \approx 0.0476$ in our adimensional units, which is in excellent agreement with the results from Garriga. Use of equation (24) above yields $T_c \approx 0.0474$, where we have used a value of R measured from the center of the bubble to the middle of the wall. The difference between the two values is well within our error stimates, and the transition is clearly seen to be first order.

The reason behind such a good agreement with the thin wall results despite the fact that the wall is only half as thick as the bubble lies in Figs.6b and 6c. In them we can see two complete periods of the solution for $T = 0.91T_c$ and $T = T_c$ respectively. We see that even at $T = T_c$ the two spheres are far from touching each other, and due to the strong exponential decay outside the wall they almost do not interact with each other at all. In these conditions the ansatz used by Garriga for obtaining Eqn.23 (namely that the action of this solution is still the action for the zero temperature bounce) is obviously still valid, thus the agreement. Finally Fig.6d shows the thermal hopping solution that becomes dominant at temperatures $T > T_c$.

The second value of f that we shall use will lay somewhere in the middle of the spectrum of possible values, at $f = 0.55$. Fig.8 shows the shape of the potential for this case, clearly away from the region where the thin wall approximation is valid. Fig.9a shows the zero temperature form of the solution (obviously already within the thick wall regime), and Figs.9b and 9c show two complete periods for $T = 0.9T_c$ and $T = T_c$. Here we can see some differences from the previous thin wall case: the two spheres collide and start merging into the wiggly cylinder structure, as shown more clearly in the aereal view depicted in Fig.9d, but at the critical temperature the solution (which in fact looks more like a "sierra" than like a cylinder) is still quite far away from the thermal hopping profile shown in Fig.9e. Finally in Fig.10 we see that, although the transition is still first order it is obviously much less strongly so that in the previous case. The same considerations about errors apply in this case as above.

The final value that we picked for f is very close to its upper possible limit, $f = 0.75$ (for $f = 0.8$ the double well structure of the potential totally disappears and we no longer have neither

a metastable state at φ_- nor, consequently, any tunneling). The shape of the potential is again depicted in Fig.11, where we see that in this case the field tunnels over a very shallow barrier. Fig.12a shows the shape of the zero temperature bounce in this case, where we can see that the thick wall features of the solution have been accentuated. Fig. 12b shows again two complete periods at $T = 0.6T_c$. We see however in this case that the term proportinal to $\partial\varphi/\partial r$ has affected the sructure of the bounces, that no longer are spherically symmetric in this case, but stretched in the τ direction. The peaks then start to interact "earlier" than in the previous cases, and at $T = 0.6T_c$ they have already stablished the wiggly cylinder or "sierra" pattern that Linde advanced. This pattern continues to develop in Figs.12c and d, where we can see how the solutions at $T = 0.96T_c$ and $T = 0.999T_c$ (the latter already inside the margin error for T_c itself) clearly and smoothly interpolate between the periodic array of bounces and the thermal hopping solution. The corresponding graph for the action is shown in Fig.13. The figure shows a typically second order transition structure, with the curve for the action of the quantum regime merging smoothly up to the second derivative into the thermal activation curve.

6   Conclusions

In this paper we have addressed the issue of whether the transition from the thermal hopping regime to the quantum regime for bubble nucleation is first or second order, in the context of field theory φ^4 phase transitions. Our main conclusion is that, whereas for most of the possible values of the parameter f that breaks the degeneracy of the two vacua the transition is first order, second order transitions will still occur when the potential barrier is sufficiently shallow.

As mentioned in the introduction, any realistic model of the field phase transition will have to incorporate a temperature dependence in the potential, the specifics of which will depend on the particular values of the parameters chosen for the model. It seems clear from our results however that any model that does not settle sufficiently rapidly in the very shallow barrier regime will most

likely present a first order transtion between the thermal and the zero temperature regime, for only very shallow barrier penetration produces the very thick bubbles that seem to be needed in order to have smooth merging of the instantons and a second order transition. Indeed, were we to expect the results from the quantum mechanical case to carry over into the the field theory problem, one could have made the point that this actually had to be the case: since in the latter situation the point at which the field exits the barrier after tunneling is still quite far away from the stable vacuum and relatively close to the metastable state, the field is not sensitive to the details of the potential beyond the barrier, and close to the true vacuum, while tunneling. In this case then one could approximate the potential by either a $-\varphi^2 + \varphi^3$ or a $-\varphi^2 + \varphi^4$ expression. However, $-q^2 + q^3$ and $-q^2 + q^4$ potentials are well known to produce second order transitions in quatum mechanics.

The main practical difference between the two cases will lay in how abruptly the quantum tunneling rate will depart from the thermally induced one in the region close to the transition temperature, first order transitions marking a much sharper deviation from the thermal hopping regime than second order ones. In the context of condensed matter physics the same instanton techniques that we have applied here have yielded predictions for decay rates of metastable states via macroscopic quantum tunneling of the system at low temperatures, and about the nature of the transition from this to the thermal activation regime, that are amenable to experimental check (i.e. [15], [16-18] among others, and more recently [19]). In this context we are likely to observe very thick wall transitions, since in most of the situations of interest in experiments we either do not have a double well structure in the potential, or have rather shallow barriers. Indeed, second order transitions have been observed in Josephson junctions, and new experiments are being prepared to study the formation of bubbles of inversed magnetization in thin films under field inversion (a process completely analogous to the one that we have studied here only that in $2 + 1$ dimensions) to check the predicted second order transition for that case.

Acknowledgements

7 References

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8 Figure Captions

Fig.1 Motion of the particle in the inverted well: a tunneling trajectory between q_1 and q_2 under the potential barrier V corresponds to a periodic motion in the inverted well $-V$ with turning points q_1, q_2.

Fig.2 (a)Monotonic dependence of β on Euclidean Energy, (b)Euclidean Action vs. Temperature $(\sim \beta^{-1})$ in this case

Fig.3 (a)Nonmonotonic dependence of β on Euclidean Energy, (b)Euclidean Action vs. Temperature $(\sim \beta^{-1})$ in this case

Fig.4 Different shapes of the instanton as temperature increases: inside the shaded regions the field attains its true vacuum value. (a) Zero Temperature bounce,(b) Periodic array of bounces at $T < 2R^{-1}$, (c) Wiggly cylinder, (d) Thermal hopping solution

Fig.5 Shape of the potential for f=0.25

Fig.6 Instantons describing the nucleation of the bubble for f=0.25. (a) $T = 0$, (b) $T = 0.91\,T_c$, (c) $T = T_c$, (d) $T \geq T_c$.

Fig.7 Temperature dependence of the Euclidean Action: $S_{min}(T)/S(0)$ versus T/T_c for $f = 0.25$.

Fig.8 Shape of the potential for $f = 0.55$

Fig.9 Instantons describing the nucleation of the bubble for f=0.55. (a) $T = 0$, (b) $T = 0.9\,T_c$,

(c) and (d) $T = T_c$, (e) $T \geq T_c$.

Fig.10 Temperature dependence of the Euclidean Action: $S_{min}(T)/S(0)$ versus T/T_c for $f = 0.55$.

Fig.11 Shape of the potential for $f = 0.75$

Fig.12 Instantons describing the nucleation of the bubble for f=0.75. (a) $T = 0$, (b) $T = 0.6\,T_c$, (c) $T = 0.90\,T_c$, (d) $T = 0.96\,T_c$, (e) $T = 0.999\,T_c$

Fig.13 Temperature dependence of the Euclidean Action: $S_{min}(T)/S(0)$ versus T/T_c for $f = 0.55$.